U.S. Department of Energy's
Office of Science

National Energy Research Scientific Computer Center (NERSC)

Advanced Scientific Computing Research
Strategic Planning workshop

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Contribution of Program Element to Overall ASCR Strategic Goal

- Most powerful unclassified computational platform
- Petascale storage facility
- Extensive client services
- Innovative software and algorithm development
- Implementing DOE grid technology

Planning horizon for Program Element

- Planning horizon is determined by a balance between
  1. Addressing the computing capability and capacity requirements of the DOE science programs
  2. Increasing the computational capability using emerging and constantly improving scientific computing technology
- Currently, achieving this balance leads to a five year program horizon

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Areas of research Program Element currently invests in

NERSC's computational resources support all SC program offices especially

- Accelerator physics
- Astrophysics
- Chemistry
- Climate and Environmental Science
- Computational Science and Mathematics
- Earth and Engineering Science
- Fusion Energy Science
- Lattice Gauge Theory
- Life Sciences
- Materials Science
- Nuclear Physics

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How does Program Element transfer knowledge or provide services to application scientists?

- Direct research collaboration on computational science projects
- Consultation in applied mathematics and computer science
- Consultation in implementing codes on massively parallel computational platforms
- Software support for a wide variety of libraries, applications, and performance tools

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How does Program Element transfer knowledge or provide services to application scientists?

- Training and instruction
- Visualization
  - Software support
  - Consultation
  - Collaboration
- Operations – maintaining a balance between high utilization and responsiveness

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Program Element Strengths

- Unparalleled, in the world, support of large-scale scientific computing by Ph. D. level scientists, mathematicians and computer scientists
- Largest unclassified computing capability
- Largest memory unclassified supercomputer in U.S.
- Largest data storage facility for SC
- Ability to procure and deploy leading-edge supercomputers

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Program Element Strengths

Partnerships

- ESnet
- Argonne National Laboratory
- Oak Ridge National Laboratory
- Pacific Northwest National Laboratory
- National Nuclear Security Administration
- U. C. Berkeley
- Mathematical Sciences Research Institute
- International Computer Science Institute
- National Aeronautics and Space Administration
- National Science Foundation
- IBM

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Program Area Weaknesses

- NERSC five year planning horizon does not appear to be meeting the requirements for computer resourced needed by
  1. Base research program
  2. SciDAC research projects
  3. INCITE
- Additional storage requirements of data intensive science are not adequately addressed
- Insufficient investment in developing and deploying new architectures for scientific computing in the production environment

Program Element Opportunities

Partnership with a computer technology vendor or vendors could accelerate deployment a new computer architecture in the production environment, in order to meet the growing demand for computational resources that has been forecast to occur over this time period.

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Program Element Threats

- If NERSC cannot keep up with the demand for computer resources, NERSC and SC will lose a large fraction of its user base as users will have to seek alternatives
- Diminished user base means a loss of scientists critical to DOE programs
- Inability to provide an exciting technological environment will lead to staff attrition
- Increased restrictive cybersecurity and (foreign) access threaten the existence of NERSC and other DOE computational facilities

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How Does the Program Element Plan?

- *Greenbook* requirements analysis (users) every three years
- Continuing technology survey and analysis
  - Advanced Systems Group
  - Future Technologies Group
  - Contact and collaborations with 1) Computational Research Division at LBNL, 2) vendors, 3) other facilities
- Periodic clean sheet planning like the 2001 5 year *Strategic Proposal* (34 pages) and the accompanying *Implementation Plan* (243 pages)

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Program Element Gap Analysis

- Disparity between the supply and demand for computational resources
- Inability to efficiently maintain and distribute mature software that has been developed within SC